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ALE3D Simulations of Gap Closure and Surface Ignition for Cookoff Modeling*

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We are developing ALE3D[1] models to describe the thermal, chemical and mechanical behavior during the heating, ignition and explosive phases of various cookoff phenomena. The candidate models and numerical strategies are being evaluated using benchmark cookoff experiments. ALE3D is a three-dimensional computer code capable of solving the model equations in a coupled fashion through all the phases of the cookoff in a single calculation. For the cookoff experiments, we are interested in representing behavior on widely varying timescales. We have used an implicit hydrodynamics option during the heating phase and an explicit solution method during the explosive phase. To complicate the modeling problem, high heat fluxes cause rapid temperature increases in boundary layers and lead to the formation of gaps between energetic and structural materials and ignition on surfaces. The initially solid energetic and structural materials react to produce gases, which fill the gaps. These materials can also melt and flow. Since an implicit solution method is used, simple no-strength materials models can no longer be used for liquids and gases. In this paper, we discuss and demonstrate choices of materials models for solid/liquid/gas mixtures to be used in conjunction with the implicit solution method. In addition, results are given for mesh movement strategies applied to the opening, closing, and surface ignition within gaps.

1. A. L. Nichols III, A. Anderson, R. Neely, and B. Wallin, Proceedings Twelfth International Detonation Symposium**, Office of Naval Research, Arlington, Virginia, ONR 333-05-2, 94, 2005.**

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Introduction

We focus on the development of a predictive capability for the violence of thermal explosion in slow and fast cookoff of energetic materials systems. This requires that we understand the fundamental reactions of energetic materials exposed to thermal stimuli and that we develop the necessary computational tools to apply this knowledge to the prediction of violence. In order to develop and refine our models, thermal explosions tests are needed that span a spectrum of explosives, case materials and violence results. Currently, the time of reaction for a specific time-temperature profile can be predicted, but reliable prediction of violence remains to be demonstrated. In order to properly assess the hazards from an event involving heating, prediction of the violence of thermal response is necessary.

Real system involve metal surface, energetic materials of variable density and porosity and intervening gaps. Furthermore, we want to investigate heating times that are very much longer than reaction timescale. This requirement means that we must use implicit hydrodynamics. It is the use of implicit hydrodynamics, in conjunction with gaps between the heated metal surface and the energetic material that we will investigate in this paper.

To demonstrate this capability, we heat LX-10 encased in a steel pipe, with a gap between the high explosive and the metal pipe. The heat transfer between the inside of the steel pipe and the surface of the high explosive is done by thermal heat conduction (thermal conductivity of air) and radiative conduction ($\varepsilon = 0.25$). We are interested in calculating the reactive violence due to the thermal heating of the LX-10 in the steel casing.

Models

Initial ALE3D simulations of the above cookoff experiment showed excellent agreement for the time to explosion and thermal profiles, but model wall expansions during the heating phase were much larger than measured values [1]. It is important to obtain accurate mechanical results during the heating phase since the mechanical state of the system at ignition has a strong effect on violence. Possible contributing factors to the above-mentioned discrepancy include the numerical errors associated with the integration of the momentum equation, the numerical representation of the gap, and errors in the chemical decomposition model. Here we focus on improvements in the integration of the momentum equation.

Most of the simulations of slow and fast cookoff with ALE3D have been calculated with explicit hydrodynamics, using courant times and time steps scaled with a technique called “mass scaling”. This is a technique that explicit dynamics codes use to

artifically raise the allowed time step above the normal Courant stability criterion. The method involves scaling the density of materials in order to decrease the effective speed of sound and therefore increase the stable Courant time step. This method applies in situations where there are many sound transient crossings during the simulation or where inertia effects are negligible. The appliciation of this methods leads to spurious oscillations in the motion of materials, and is numerically inefficient. There is an effort in progress to develop the implicit method of integration to the point where cookoff problems can be accurately modeled.

Recently, several improvement have been made in the implicit hydrodynamics algorithm in ALE3D so that cookoff simulation can be performed. For the mechanical modeling of soft materials, the one-point quadrature used in numerical integration was replaced by an eight-point quadrature routine to improve numerical stability. This improvement is being applied for two numerical treatments of dynamic gaps between the explosive and case: mixed materials and slide surfaces. For the case of mixed materials the boundary between the explosive and air is not tracked with the mesh, resulting in some numerical zones with both explosive and air. This approach avoids mesh tracking difficulties and will work well with cases involving the flow of HE decomposition gases into the air gaps and through vents and leaks in the case to the outside environment. The disadvantages are that this approach does not currently accomodate thermal radiation across the gap and does not efficiently track the air/HE interface. Currently, work is focused on the development of a gap material for use with the implicit integration scheme for the momentum equation. A material for one-dimensional gap closing has been developed and will be extended to treat the case of more complex gap shapes.

The second method to treat gaps involves the method of slide surfaces in which air/gap interface is tracked with the mesh and there is no gap material. Although thermal radation across the gap is treated, it does not readily accomodate the flow of HE decomposition gases in the gap. Also there are questions about the practicality of using the method of slide surfaces in highly complex geometries. To date the eight-point quadrature and gap closing algorithms have been installed for slide surfaces. Work is in progress to add friction needed for multidimensional problems. Here we present a demonstration problem for slow cookoff.

Consider the slow cookoff of LX-10 (HMX, 95%, and VITON, 5%), in a 1D STEX vessel (see Figures 6 and 7). The vessel is made of 4130 steel, has a 5.08 cm ID and a wall thickness of 0.406 cm. The decomposition of LX-10 is represented by a multi-step reaction model and a power-law expression is used to represent the laminar burn of the HE after ignition. Standard models are used for the strength and equation of state of the LX-10 solid and gas species, air, and steel [4]. The surface temperature of the vessel is increased at the rate of 2^{o}C/hr for 100 hours. The method of slide surfaces is used to represent the closing of a 0.2 mm gap between the steel and the outside radius of the HE. The gap closes as the HE expands inside the steel due to thermal expansion and the formation of decomposition gases.

The temperature in the HE at the axis of symmetry is close to the steel temperature until self heating and ignition occur (see Figure 7a). The hoop strain at the outside steel surface increases monotonically, accelerating first with the closing of the gap at approximately $1x10^{5}$ seconds, the formation of decomposition gases, and finally the ignition and deflagration of the HE (see Figure 7b). The same simulation with twice

the number of zones in each coordinate direction gave a nearly identical curve, indicating mesh convergence for a small number of zones. The oscillations characteristic of the mass-scaling approach are absent. Also the mesh convergence is much faster for the implicit approach. The next steps are to add friction for the slide surface approach, and complete the gap material models for the mixed material method.

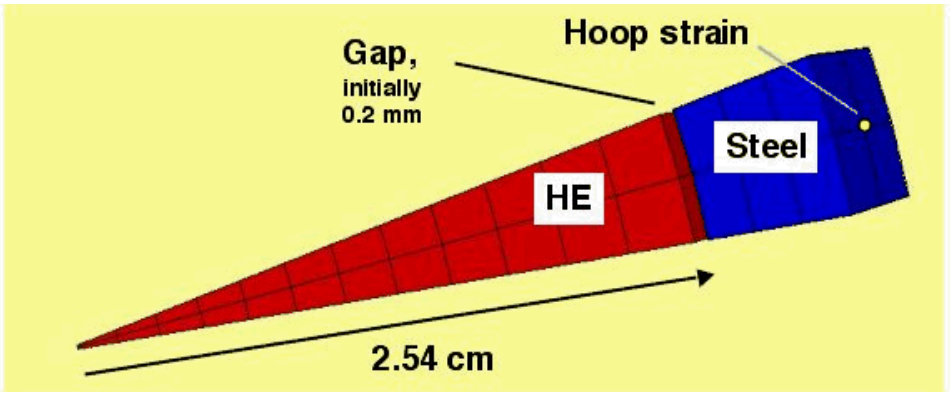


Figure 6. 2D cylindrical wedge mesh with theLX-10, gap, and 4130 steel. The temperature of the surface of the steel is increased at the rate 2 °C per hour.

ALE3D chemical, mechanical and thermal modes have been developed to model the cookoff of LX-10 in the STEX test. The decomposition of HMX in the LX-10 is modeled by a four-step, five species chemical kinetics model. The first two steps are endothermic and the final two steps are exothermic as indicated in Table 1.

$A \rightarrow B \qquad r_1 = Z_1 \exp(-E_1/RT)\rho_A \qquad (2)$

$B \rightarrow C \qquad r_2 = Z_2 \exp(-E_2/RT)\rho_B \qquad (3)$

$C \rightarrow D \qquad r_3 = Z_3 \exp(-E_3/RT)\rho_C \qquad (4)$

$D \rightarrow E \qquad r_4 = Z_4 \exp(-E_4/RT)\rho_D^2 \qquad (5)$

We assume that the VITON A does not decompose until the LX-10 reaches the deflagration state. Here ρ_I is the mass concentration of a reactant i. The quantities r_i, Z_j and E_j are the reaction rate, frequency factor and activation energy, respectively, for a reaction j. The components A and B are the solid species β- and δ-HMX, C is a solid intermediate and D and E are intermediate and final gas products. The determination of the chemical kinetic parameters of Table 1 are described below.

Table1

Reaction sequence	Reaction Step	Ln Z_i	E_i (KJ/g-mole-K)	Q_k (J/g)
HMX	A → B	48.13 s^{-1}	202.70	41.88 (endothermic)
	B → C	48.70 s^{-1}	220.39	209.38 (endothermic)
	C → D	37.80 s^{-1}	185.26	-808.21 (exothermic)
	D → E	28.10 cm^3/s-g	142.60	-6155.75 (exothermic)

Table 2

	ρ (g/cm^3)	C_v(J/kgK)	Thermal conductivity (W/mK)
HMX_A	1.865	2185.	0.456
HMX_B	1.755	2048.	0.456
HMX_C	1.755	2048.	0.456
HMX_D	1.865	1422.	0.1317
HMX_E	1.865	1422.	0.1317
VITON_A	1.865	2185.	0.456

After the Arrhenius reaction rates have increased to the point where changes are occurring on the time scale of sound propagation, a switch is made to a burn model in which the reactants are converted to products in a single reaction step. This switch in models is made for two reasons. The first is that the computational capabilities and methods are not yet available to resolve reaction zones which can be on the time scale of $1\text{-}10^4$ s in the ODTX apparatus may not apply on shorter time scales. It is likely that deflagration rates measured in the strand burner provide a better measure of reaction behavior on short time scales. We assume that the burn front velocity, V, is a function of the pressure, P, at the front location, and use power-law expressions of the form to describe segments of the burn front curve:

$$V = V_o(p/p_o)^n$$

Here the subscript 0 indicates a reference quantity.

The mechanical behavior of the condensed high-explosive constituents (HMX_A, HMX_B, HMX_C) along with the Viton reactant (Viton_A) are represented by Steinberg-Guinan mechanical models with a 7-terms polynomial equation of state. The density and thermal properties of these species are given in Table 2. The constant volume

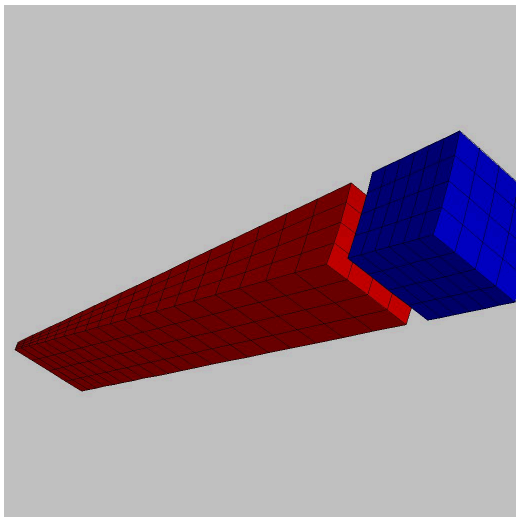
heat capacity does not vary with temperature. Calculated melt and cold curves are used to account for the influence of compression on melting energy. A nonlinear regression procedure was used to determine the coefficients that give an optimal representation of the measurements of the thermal expansion, compressibility, sound speed and the unreacted shock Hugoniot.

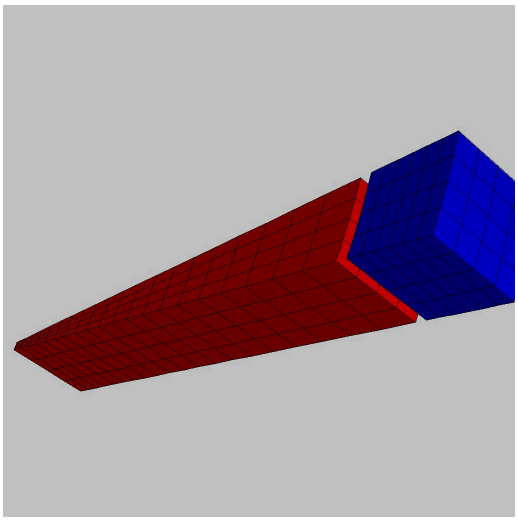
The model gas constituents (HMX_D, HMX_E, ITON_B) along with the air in the gap are treated as no-strength materials with gamma-law equations of state. This equation of state provides an approximate representation over much of the pressure range, except at the higher pressures of 10 kbar where the model is less accurate. The Γ-value for the HE gas species is set using a pressure of 1 kbar, a temperature of 2273K and the density and heat capacity from the thermo-chemical equilibrium computer code, CHEETAH 4.0 for the final product gases.

The time-dependent thermal transport model includes the effects of conduction, reaction, advection, and compression. The constant-volume heat capacity is constant for each reactant consistent with the Steinberg-Guinan model. The thermal conductivity for the condensed species A and B are taken to be constant, whereas the effects of temperature are included for the gaseous species. The heat capacity for the gases is assigned the same constant-volume value used in the gamma-law model. The temperature dependent thermal conductivity is estimate at 1 kbar using Bridgman's equation for liquids in which the sound velocity is calculated using results from CHEETAH.

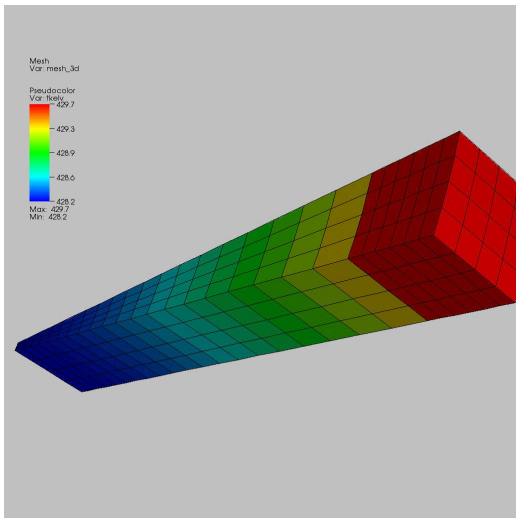
The ALE3D computer code requires 3D meshes, and a wedge-shaped mesh is employed for the 2-D model of this study, A small hole is present near the symmetry axis to allow the use of hexahedral elements at all locations. In the base case, the tube cavity has 12 elements in the radial direction, which is increased by a factor of 2 in mesh refinement studies. Some of the elements have both HE and air, and standard mixing rules are employed to calculate the energy, heat capacity, thermal conductivity , shear modulus and equation of state. The mesh is smoothed using a combination of Lagrange and Eulerian algorithms. Nodes initially on the interface between the cavity and the steel remain on these boundaries while nodes interior to the cavity are advected through the flowing HE and air.

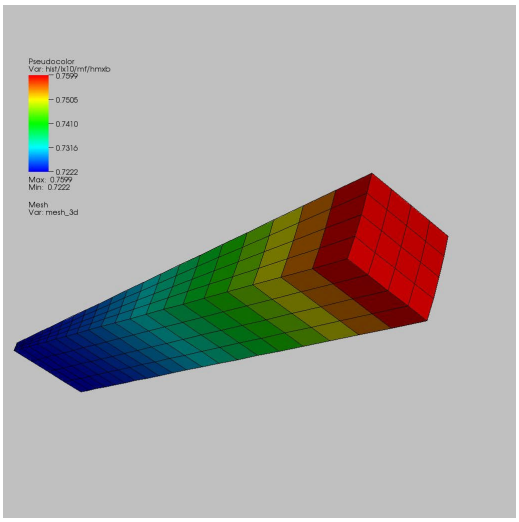
Results



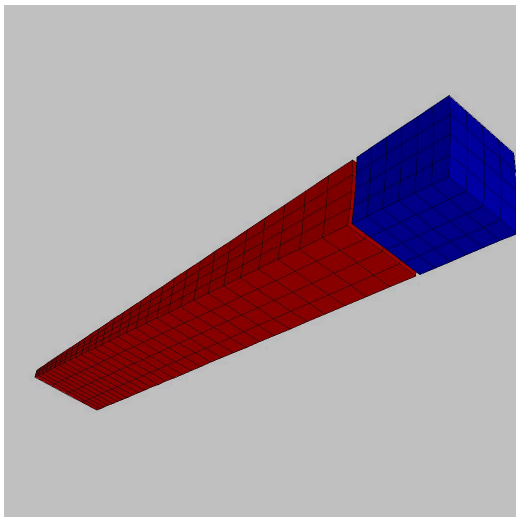


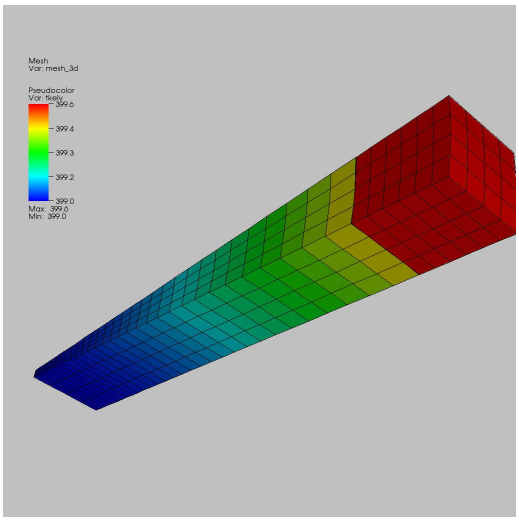
The grid at initial time with an 1.0 mm gap, using slide surfaces. At a time of 61.6 hours the gap has been reduced to 0.5 mm.



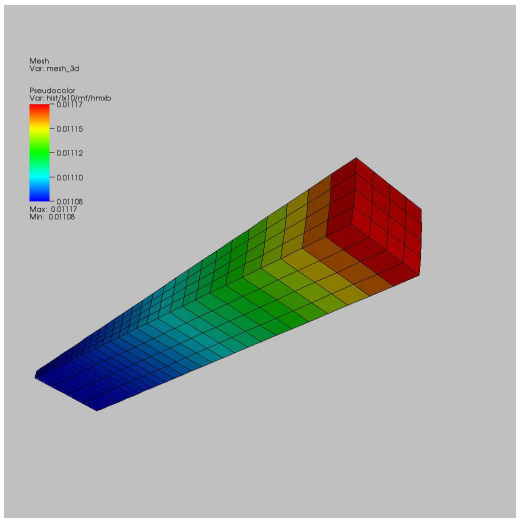


The gap closes at a time 65.8 hours, where the temperature distribution is nearly uniform at 430K. At this temperature most of the β-HMX has been transformed to δ-HMX. The deflagration temperature has been set to a temperature 700K.

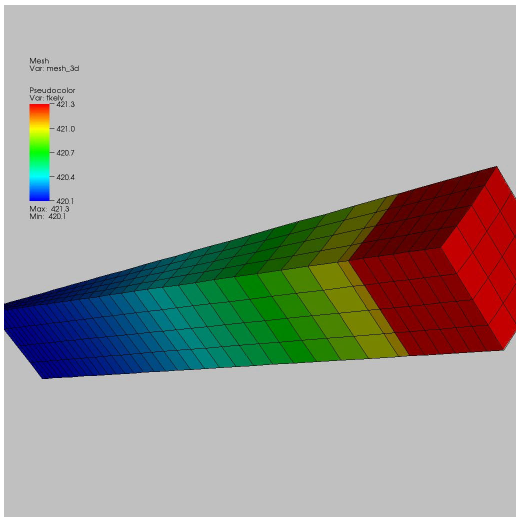




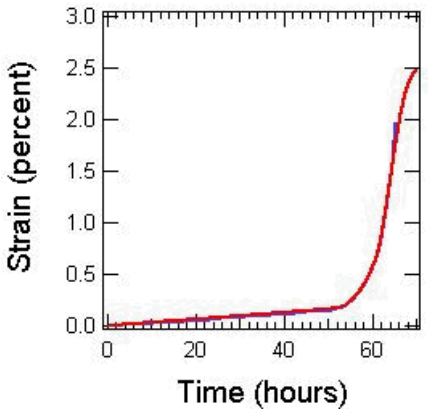
The grid at initial time with 0.2 mm gap, using slide surfaces. The temperature when the gap closes at 50.8 hours is approximately 400K.



When the gap closes in this case only a small amount of β-HMX was been transformed to δ-HMX.



With the material model for air in the gap, we also calculate the 1.0 mm gap to close to 0.5 mm in 61.6 hours. At this time the temperature is nearly uniform at 420 K.



The hoop strain of the steel during the slow heating is identical for both gap methods with an initial gap of 0.2 mm

Conclusions

We have calculated slow cookoff heating (2 C/hr) for the case where LX-10 is encased in steel, with a large (1.0 mm) or small gap (0.2 mm) between the high explosive and the steel. In both cases we are able to calculated the closing of the gap by thermal expansion and chemistry of making gaseous products from the reacting high explosive. We are able to flow multiple phases of the HMX chemistry.

References

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